GABS v11.0 Program Manual

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(Dated: January 20, 2015)

This code and documentation is based on the version (10, February 2011) by Edgardo Browne (Lawrence Berkeley National Laboratory). The original code was adapted for IBM PC by Coral M. Baglin (Lawrence Berkeley National Laboratory) in September 1991.

I. INTRODUCTION

GABS calculates absolute gamma-ray intensities and a decay-scheme normalization factor (NR) for converting relative intensities to absolute values per 100 decays of the parent nucleus. Decay mode branching ratios (BR) for radionuclides that decay through several decay modes are also determined, along with the uncertainties for all of these quantities. The nature of the physical problem and the mathematical formulas used here are described elsewhere [1].

II. TECHNICAL SPECIFICATIONS

GABS consists of a main program (GABS), a subroutine GAMMAS, a few functions, and NSDFLIB, a package of character-string functions and subroutines maintained by the Brookhaven National Laboratory. The program, was originally written in FORTRAN 77 for a VAX-11/8600 computer with the VMS operating system, and was later adapted for IBM PC. The present version of GABS has been updated for FORTRAN 90.

GABS prompts the user for a file name of an input data set, and writes the results of the calculation on a report file (default name: GABS.RPT). Output data set of the calculation can also be created in ENSDF format, written to a file (default name: GABS.NEW). The user may specify the name of each of these files.

An input file name (say 127Te.in) can also be passed on the command line by entering "gabs 127Te.in". The program will create a report file (127Te.rpt) and new ENSDF file (127Te.new). Sample terminal dialogue is shown in Fig. 1.

```
C:\ENSDF_codes\Gabs\Test>gabs
 ===========  GABS Version 11 [15-Dec-2014]  ===========
GABS: Enter input file name: 127Te.in
GABS: Enter REPORT FILE name (def=GABS.rpt): 127Te.rpt
GABS: Do  you want to create a new data set? (N/Y): y
GABS: Enter file name for new ENSDF dataset (def=GABS.new): 127Te.new

Calculations completed
ENSDF input file: 127Te.in
Report file:      127Te.rpt
new ENSDF file:   127Te.new

C:\ENSDF_codes\Gabs\Test>gabs 127Te.in
 ===========  GABS Version 11 [15-Dec-2014]  ===========

Calculations completed
ENSDF input file: 127Te.in
Report file:      127Te.rpt
new ENSDF file:   127Te.new

C:\ENSDF_codes\Gabs\Test>
```

FIG. 1: Terminal dialogue of GABS – top: interactive use; bottom: batch use by passing input file on the command line.

GABS will give some error messages if filenames or input parameters are incorrect – strongly recommended that the input files are checked by means of FMTCHK.

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The program was compiled with Intel FORTRAN compiler and distributed as binary executables for Windows, Linux and Mac OS operating systems. The source code and sample input, output and report files (see section IV) are also included.

III. INPUT DATA

GABS reads up to three data sets in ENSDF format [2]. A blank (END) record should follow each data set including the last one. The user must supply the following additional information:

N-RECORD The fraction (NB) of the decay intensity carried by the γ rays, in columns 42-49, and corresponding uncertainty (DNB) in columns 50-51 are used for normalize the decay scheme. Both quantities should be given in ENSDF style: for example, 0.934 21 means 0.934 $\pm$ 0.021. Default values assigned by the program are NB=1.0 and DNB=0.0. Input values for the branching ratio (BR), in columns 32-39, and uncertainty (DBR) in columns 40-41 are used for single-data set calculations. Default values assigned by the program are BR=1.0 and DBR=0.0. Alphanumeric data are not acceptable in the uncertainty fields DG or DBR. A character "C" in column 80 tells the program that the γ rays belong to a cascade and that they carry the full transition intensity (i.e., there are no direct β^-, β^+ or EC feedings to intermediate levels). When carrying out multiple data set calculations (for which the program calculates the branching BR), the BR fields must be blank in all data sets.

G-RECORD All γ-ray transitions used in the calculation of the normalization factors must be identified with an "X" or a "Y" in column 79, as described below:

"X" – if DRI is blank, the program assigns 20% uncertainty to the relative γ-ray intensity,

"Y" – the original value of DRI, including a blank, will be used in the calculations.

GABS does not use the total-intensity field (TI) in columns 65-74 in the calculation, one could make use of reported total transition intensities (photons + conversion electrons) by moving them to the relative-photon field (RI) in columns 22-29. Their uncertainties should be correspondingly moved and the conversion coefficients (CC) set to 0 (columns 56-62 blank). However, the output file should be edited at the end to restore the records to their original form.

The following character strings are acceptable in the uncertainty fields (DRI):

CA (calculated) – translated to represent 50% uncertainty, although carefully estimated input uncertainties are far more preferable to arbitrarily assigned 50% values.

AP (approximate) – translated to represent 50% uncertainty.

LT - (less than) – translated to $RI/2 \pm RI/2$.

Since the program ignores all comment (CG) and continuation (2 G, 3 G) records, users should not include any input data needed by GABS in this types of record.

IV. CALCULATIONS AND SAMPLE CASES

The program is distributed with three sample input files: 127Te.in (single data set), 176Lu.in (single data set with cascade γ rays) and 80Br.in (multiple data set) in which the total conversion coefficients have been updated by means of BrIcc v2.3a (10-Dec-2014). Data input, ENSDF output and report files for these examples are presented below in Figs. 2, 3, 4 (^{127}Te); 5, 6, 7 (^{176}Lu) and 8, 9, 10 (^{80}Br). Absolute γ-ray intensities and uncertainties given in parentheses are the values calculated assuming that the relative γ-ray intensities and NR are independent quantities. These uncertainties for weak γ rays are very close to those calculated without adopting such an assumption, and therefore the user may remove their corresponding %IG comment records from the ENSDF data set. Uncertainties in the intensities of the γ rays not used in the calculation of NR are determined by combining the uncertainty in the relative intensity in quadrature with the uncertainty in the normalization factor ($NR \times BR$).

A. Single Data Set

GABS calculates the normalization factor NR and uncertainty DNR, as well as the uncertainties in the absolute γ-ray intensities.

```
127I      127TE B- DECAY (9.35 H)
127I   N                                0.012   2
127TE  P        0.0  3/2+                9.35 H 7                    694 5
127I   L        0.0  5/2+              1.0E+10 YGT
127I   B                99                    6
127I   L    57.609 117/2+                1.95 NS 1
127I   G 57.609    11     3.0 3M1+E2     0.084   6     3.72                  X
127I   L    202.859 83/2+
127I   G 145.250   9   0.338 16E2                    0.471
127I   G 202.859   8    5.85 21M1+E2     0.52    5     0.1143 22             X
127I   B                 0.03                  9
127I   L    374.990 91/2+
127I   G 172.131   8   0.035 APM1+E2     0.084   7     0.1649 24
127I   G 374.989   9   0.023 APE2                    0.0199                X
127I   B               6.E-04                10
127I   L     417.93 65/2+
127I   G 215.07    6    3.91 17M1+E2     0.203   15    0.0911
127I   G 360.32    6     13.6 3M1+E2     0.194   15    0.0233
127I   G 417.93    6     100 10M1+E2     0.08    3     0.01599               X
127I   B               1.2                   6
127I   L      618.4 3(3/2)+
127I   G 618.4     3    0.013 2M1+E2                   0.0055 7              X
127I   B              1.3E-04                8
```

FIG. 2: Sample input file (127Te.in) of single data set.

```
127I      127TE B- DECAY (9.35 H)
127I   N   0.0098  19             1.00
127TE  P        0.0  3/2+                9.35 H 7                    694 5
127I   L        0.0  5/2+              1.0E+10 YGT
127I   B                99                    6
127I   L    57.609 117/2+                1.95 NS 1
127I   G 57.609    11     3.0 3M1+E2     0.084   6     3.72
127I  CG           %IG=0.029  6, using the calculated normalization.
127I   L    202.859 83/2+
127I   G 145.250   9   0.338 16E2                    0.471
127I  CG           %IG=0.0033  7, using the calculated normalization.
127I   G 202.859   8    5.85 21M1+E2     0.52    5     0.1143 22
127I  CG           %IG=0.057 11, using the calculated normalization.
127I   B                 0.03                  9
127I   L    374.990 91/2+
127I   G 172.131   8   0.035 APM1+E2     0.084   7     0.1649 24
127I  CG           %IG=0.00034 19, using the calculated normalization.
127I   G 374.989   9   0.023 APE2                    0.0199
127I  CG           %IG=0.00023 12, using the calculated normalization.
127I   B               6.E-04                10
127I   L     417.93 65/2+
127I   G 215.07    6    3.91 17M1+E2     0.203   15    0.0911
127I  CG           %IG=0.038  8, using the calculated normalization.
127I   G 360.32    6     13.6 3M1+E2     0.194   15    0.0233
127I  CG           %IG=0.13  3, using the calculated normalization.
127I   G 417.93    6     100 10M1+E2     0.08    3     0.01599
127I  CG           %IG=0.98 19, using the calculated normalization.
127I   B               1.2                   6
127I   L      618.4 3(3/2)+
127I   G 618.4     3    0.013 2M1+E2                   0.0055 7
127I  CG           %IG=0.00013  3, using the calculated normalization.
127I   B              1.3E-04                8
```

FIG. 3: Sample ENSDF output file for single data set.

```
* * * GABS Version 11 [15-Dec-2014] Report file  * * *
      Current date: 12/15/2014
      ENSDF input file: 127te.in
      new ENSDF file:   127te.new

      Data Set:  127TE B- DECAY (9.35 H)
      NR=    0.0098  19     BR=    1.00

      E= 57.609    11 %IG=0.029  6 per 100 dis. Compare with 0.029  7
      E= 145.250   9  %IG=0.0033  7 per 100 dis.
      E= 202.859   8  %IG=0.057 11 per 100 dis. Compare with 0.057 11
      E= 172.131   8  %IG=0.00034 19 per 100 dis.
      E= 374.989   9  %IG=0.00023 12 per 100 dis. Compare with 0.00023 12
      E= 215.07    6  %IG=0.038  8 per 100 dis.
      E= 360.32    6  %IG=0.13  3 per 100 dis.
      E= 417.93    6  %IG=0.98 19 per 100 dis. Compare with 0.98 21
      E= 618.4     3  %IG=0.00013  3 per 100 dis. Compare with 0.00013  3
```

FIG. 4: The calculation report file for single data set.

B. Single Data Set with Cascade γ rays

GABS calculates the normalization factor (NR) and uncertainty (DNR), as well as the uncertainties in the absolute γ-ray intensities. The program normalizes the sum of the transition intensities of K cascade γ rays to $(100 \times K \times BR \times G)$. Since there are three cascade γ rays in the example shown below (K=*3*), GABS normalizes the sum of the transition intensities to 300.

```
176HF    176LU B- DECAY
176LU  P 0.0         7-               4.00E10 Y 22             1192.8    9
176HF  N                       1.0       1.0                                 C
176HF PN                                                                   3
176HF  L    0.0      0+
176HF  L   88.36    42+
176HF  G 88.36     4 14.1    14E2                     5.77                  X
176HF  L  290.19    64+
176HF  G 201.83    4 90.8    50E2                     0.279                 X
176HF  L  597.03    76+
176HF  G 306.84    4 100       E2                     0.0740                Y
176HF  L  998.13   228+
176HF  G 401.1     2 0.35    2 E2                     0.0345
```

FIG. 5: Sample input (176Lu.in) file for single data set with cascade γ rays.

```
176HF    176LU B- DECAY
176LU  P 0.0         7-               4.00E10 Y 22             1192.8    9
176HF  N     0.94   4              1.00
176HF PN                                                                   3
176HF  L    0.0      0+
176HF  L   88.36    42+
176HF  G 88.36     4 14.1    14E2                     5.77
176HF CG           %IG=13.3 10, using the calculated normalization.
176HF  L  290.19    64+
176HF  G 201.83    4 90.8    50E2                     0.279
176HF CG           %IG=85  4, using the calculated normalization.
176HF  L  597.03    76+
176HF  G 306.84    4 100       E2                     0.0740
176HF CG           %IG=94  4, using the calculated normalization.
176HF  L  998.13   228+
176HF  G 401.1     2 0.35    2 E2                     0.0345
176HF CG           %IG=0.329 23, using the calculated normalization.
```

FIG. 6: Sample ENSDF output file for single data set with cascade γ rays.

C. Multiple Data Sets

GABS calculates for each data set the branching ratio BR and uncertainty DBR, the γ-ray normalization factor NR, and the uncertainties in the absolute γ-ray intensities. Notice that NR and BR are not independent quantities for a decay scheme with two or more decay modes. Therefore, the relevant uncertainty for the branching ratio is that of BR, and for the absolute γ-ray intensities are of the form $BR \times NR$.

```
* * * GABS Version 11 [15-Dec-2014] Report file - cascade gamma rays  * * *
      Current date: 12/15/2014
      ENSDF input file: 176Lu.in
      new ENSDF file:   176Lu.new

      Data Set: 176LU B- DECAY
      NR=      0.94   4     BR=    1.00

      E= 88.36     4  %IG=13.3 10 per 100 dis. Compare with 13.3 14
      E= 201.83    4  %IG=85  4 per 100 dis. Compare with 85  6
      E= 306.84    4  %IG=94  4 per 100 dis. Compare with 94  4
      E= 401.1     2  %IG=0.329 23 per 100 dis.
```

FIG. 7: Calculation report file for single data set with cascade γ rays.

```
80SE    80BR EC DECAY (17.68 M)
80SE  N                                0.145       12
80BR  P    0.0       1+               17.68 M      2           1870.3 20
80SE  L    0.0       0+
80SE  E                2.17 22  4.9    5   4.7      1              7
80SE  L  665.94   15 2+
80SE  G 665.94    15  16.1  14E2                    1.19E-3                X
80SE  E                        1.1        4.9      1              1.1
80SE  L 1448.9     3 2+                                                     ?
80SE  G 783.0     3    0.1  APE2+M1                  0.000707               ?
80SE  G 1448.9    3    0.24 LTE2                     2.54E-4                X
80SE  E                       0.02  LE   6        GT              0.02LE
80SE  L 1477.4     5 0+
80SE  G 811.4     5    0.6  2 (E2)                   7.03E-4
80SE  E                       0.05   2   5.3      3              0.05 2

80KR    80BR B- DECAY (17.68 M)
80KR  N                                0.073       8
80BR  P    0.0       1+               17.68 M      2           2006   11
80KR  G  677.6    10   0.12  4                                             ?
80KR  G  688.0    10   0.18  5                                             ?
80KR  G 1339.1     8
80KR  L    0.0       0+
80KR  B 1997      10  85.0   7              6
80KR  L  616.9     3 2+
80KR  G 616.9     3  100    10E2                    1.72E-3                X
80KR  B 1380      20   6.2   6              6.0      1
80KR  L 1256.8     3 2+
80KR  G 639.93    18   3.8   3E2+M1     6       1     1.54E-3
80KR  G 1256.8     3   1.18 10                                             X
80KR  B                0.31  3              6.3      1
80KR  L 1321.2     3  0(+)
80KR  G 704.37    19   2.9   4(E2)                   1.19E-3
80KR  B                0.19  2              6.4      1
```

FIG. 8: Sample input (80Br.in) file for multiple data set.

[1] **1986Br21** E. Browne, *Calculated Uncertainties of Absolute γ-ray Intensities and Decay Branching Ratios Derived from Decay Schemes*, Nucl. Instr. Meth. **A249** (1986) 462; http://dx.doi.org/10.1016/0168-9002(86)90703-5

[2] **2001TuZZ** J.K. Tuli, *Evaluated Nuclear Structure Data File A Manual for Preparation of Data Sets*, BNL-NCS-51655-01/02-Rev, National Nuclear Data Center, Brookhaven National Laboratory; http://www.nndc.bnl.gov/nndcscr/documents/ensdf/ensdf-manual.pdf

```
80SE    80BR EC DECAY (17.68 M)
80SE  N     0.89                0.075 9
80BR  P    0.0       1+               17.68 M       2            1870.3 20
80SE  L    0.0       0+
80SE  E                2.17 22  4.9    5   4.7       1               7
80SE  L  665.94   15 2+
80SE  G 665.94    15  16.1  14E2                     1.19E-3
80SE CG           %IG=1.07 13, using the calculated normalization.
80SE  E                       1.1        4.9       1               1.1
80SE  L 1448.9     3 2+                                                    ?
80SE  G 783.0     3    0.1  APE2+M1                  0.000707              ?
80SE CG           %IG=0.007  4, using the calculated normalization.
80SE  G 1448.9    3    0.24 LTE2                     2.54E-4
80SE CG           %IG=0.008  8, using the calculated normalization.
80SE  E                       0.02  LE   6        GT              0.02LE
80SE  L 1477.4     5 0+
80SE  G 811.4     5    0.6  2 (E2)                   7.03E-4
80SE CG           %IG=0.040 14, using the calculated normalization.
80SE  E                       0.05   2   5.3       3               0.05 2

80KR    80BR B- DECAY (17.68 M)
80KR  N    0.072                0.925 9
80BR  P    0.0       1+               17.68 M       2            2006   11
80KR  G  677.6    10   0.12  4                                             ?
80KR CG           %IG=0.008  3, using the calculated normalization.
80KR  G  688.0    10   0.18  5                                             ?
80KR CG           %IG=0.012  4, using the calculated normalization.
80KR  G 1339.1     8
80KR  L    0.0       0+
80KR  B 1997      10  85.0   7              6
80KR  L  616.9     3 2+
80KR  G 616.9     3  100    10E2                     1.72E-3
80KR CG           %IG=6.7  7, using the calculated normalization.
80KR  B 1380      20   6.2   6              6.0      1
80KR  L 1256.8     3 2+
80KR  G 639.93    18   3.8   3E2+M1     6       1     1.54E-3
80KR CG           %IG=0.25  3, using the calculated normalization.
80KR  G 1256.8     3   1.18 10
80KR CG           %IG=0.079 10, using the calculated normalization.
80KR  B                0.31  3              6.3      1
80KR  L 1321.2     3  0(+)
80KR  G 704.37    19   2.9   4(E2)                    1.19E-3
80KR CG           %IG=0.19  4, using the calculated normalization.
80KR  B                0.19  2              6.4      1
```

FIG. 9: Sample ENSDF output file for multiple data set.

```
 * * * GABS Version 11 [15-Dec-2014] Report file  * * *
       Current date: 12/15/2014
       ENSDF input file: 80br.in
       new ENSDF file:   80br.new

       Data Set: 80BR EC DECAY (17.68 M)
       NR=      0.89         BR=   0.075   9

       E= 665.94    15 %IG=1.07 13 per 100 dis. Compare with 1.07 19
       E= 783.0     3  %IG=0.007  4 per 100 dis.
       E= 1448.9    3  %IG=0.008  8 per 100 dis. Compare with 0.008  8
       E= 811.4     5  %IG=0.040 15 per 100 dis.

       Data Set: 80BR B- DECAY (17.68 M)
       NR=     0.072         BR=   0.925   9

       E=  677.6    10 %IG=0.008  3 per 100 dis.
       E=  688.0    10 %IG=0.012  4 per 100 dis.
       E= 616.9     3  %IG=6.7  7 per 100 dis. Compare with 6.7  9
       E= 639.93    18 %IG=0.25  3 per 100 dis.
       E= 1256.8     3 %IG=0.079 10 per 100 dis. Compare with 0.079 10
       E= 704.37    19 %IG=0.19  4 per 100 dis.
```

FIG. 10: Sample calculation report file for multiple data set.